Improved two-dimensional dynamic batch process monitoring with support vector data description

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Abstract: For dynamic batch process monitoring, a two-dimensional dynamic modeling framework has recently been formulated, which is based on a two-dimensional autoregressive model and the principal component analysis (PCA) method. Different from traditional dynamic batch process monitoring, the two-dimensional method can monitor both within batch and batch-to-batch dynamic information of the process data. However, this PCA-related method has two main restrictions, which may render poor monitoring performance in practice. First, it is under the assumption that the distribution of the process data is Gaussian. Second, the correlations between different process variables are assumed to be linear with each other. Unfortunately, both of these two assumptions are difficult to satisfy in batch processes. In this paper, support vector data description (SVDD) is incorporated into the two-dimensional modeling framework, which has no Gaussian limitation of the data, and can also model the nonlinear relationship between process variables. For dynamic batch process monitoring, a distance based statistic is proposed. Based on results of a simulation case study, the monitoring performance has been improved.

1. INTRODUCTION

Batch processes play an important role in producing low volume and high value-added chemical and biochemical products. To ensure operation safety and quality consistency in batch processes, online monitoring and quality prediction are both important. Conventional multivariate statistical process control (MSPC) methods such as principal component analysis (PCA) and partial least squares (PLS), which were successfully used for continuous process monitoring, have been extended for batch process monitoring, for example, multiway PCA, multiway PLS, phase or stage based method and etc [Nomikos, and MacGregor, 1994, 1995; Chen, and Chen, 2006; Sprang et. al., 2008; Yao, and Gao, 2009b; Camacho et. al., 2009]. Recently, the dynamic behavior of the batch process has been explored, and corresponding monitoring methods have been developed. For example, Chen and Liu proposed batch dynamic PCA and batch dynamic PLS for process monitoring [Chen, and Liu, 2003]. Floreses-Cerrillo and MacGregor proposed a dynamic batch process monitoring method based on the batch-to-batch information [Floreses-Cerrillo, and MacGregor, 2004]. Lee and Dorsey proposed a state-space model for batch process monitoring [Lee, and Dorsey, 2004]. Fletcher et al. proposed a local dynamic PLS approach for modeling batch process [Fletcher et. al., 2008]. Jia et al. proposed a online batch dynamic monitoring method by introducing the dynamic data information into the kernel PCA method [Jia et. al., 2010].

However, most of those developed methods have only considered one-dimensional batch dynamic information of the process, either the time-wise dynamic or the batch-wise dynamic. Actually, the dynamic behavior of the batch process may exist not only within a batch, but also from batch to batch. To this end, a two-dimensional batch dynamic monitoring approach has been proposed [Lu et. al., 2005; Yao, and Gao, 2008, 2009a]. By combining PCA with the two dimensional autoregressive model structure, the dynamic information of both two dimensions can be efficiently modeled and used for batch process monitoring. However, this PCA related method is under assumptions that the data distribution is Gaussian and the correlations between different process variables are linear, both of which are difficult to satisfy in batch processes.

This paper aims to incorporate a one-class classification method into the two-dimensional batch dynamic monitoring framework, which is called support vector data description (SVDD). SVDD was originally proposed by Tax et al. for the one-class classification problem [Tax, and Duin, 1999], such as damage detection, image classification, one-class pattern recognition, and etc [Tax, and Duin, 2004]. In fact, batch process monitoring can also be considered as a one-class classification problem, since the aim of monitoring is to separate the normal process data samples from the faulty ones. Compared to the PCA based method, SVDD has no Gaussian limitation of the process data, and also can model the nonlinear correlation between process variables. Recently, SVDD has been incorporated into several traditional multivariate statistic modeling methods for continuous process monitoring [Liu et. al., 2008; Ge et. al., 2009]. However, it has not been used for batch process monitoring up to now, especially for dynamic batch process monitoring. By incorporating the SVDD model for two-dimensional dynamic batch process monitoring, both of two restricted assumptions can be eliminated.

The remainder of this paper is organized as follows. In section 2, the SVDD model is incorporated into the two-dimensional dynamic batch process monitoring framework. A simulation case study on a two-dimensional batch process is provided for performance evaluation of the proposed
methods in section 3. In the last section, some conclusions are made.

2. INCORPORATION OF SVDD FOR TWO-DIMENSIONAL DYNAMIC BATCH PROCESS MONITORING

2.1. Two-dimensional data structure of the batch process

Conventionally, the dataset of the batch process is collected through a three-way manner $X(I \times J \times K)$, where $I$ is the batch number, $J$ is the variable number, and $K$ is the total number of data samples within each batch. In the case of batch processes with two-dimensional dynamics, the current value of each process variable $x_{i}(k), j = 1, 2, \cdots J$ is not only correlated with the past values in time direction $x_{i}(k-1), x_{i}(k-2), \cdots x_{i}(k-p)$ within the batch, but also related with the past values in the batch direction $x_{i}(i-1,k), x_{i}(i-2,k), \cdots x_{i}(i-q,k)$, where $p$ and $q$ are the autoregressive orders in the two directions, respectively. Besides, $x_{i}(k)$ may be also correlated with the past values in the crossed time and batch directions.

For two-dimensional dynamic batch process modeling, an augmented data matrix is defined, which can simultaneously incorporate the dynamic information in both two directions. However, before generating this augmented data matrix, two important parameters should be determined for each process variable, which are the dynamic orders in the two directions $p$ and $q$. In the previous work, the region which included the two-dimensional dynamic information was defined as the region of support (ROS) [Lu et al., 2005]. Different methods have been proposed to determine the ROS parameters, such as two-dimensional Akaike information criterion, backward elimination method, and iterative stepwise regression method. In the present work, the two-dimensional Akaike information criterion based method is used for determining the two parameters $p$ and $q$ in the batch process.

By defining $x_{i}(k) = [x_{i}(i,k), x_{i}(i,k), \ldots x_{i}(i,k)]$ for the $k$-th time slice in the $i$-th batch, the augmented data matrix can be formulated as follow

$$X_{\text{aug}} = \begin{bmatrix}
X_{i}(q+1,p+1) & X_{i}(q+1,p+2) & \cdots & X_{i}(q+1,K) \\
X_{i}(q+1,p+1) & X_{i}(q+1,p+2) & \cdots & X_{i}(q+1,K) \\
\vdots & \vdots & \ddots & \vdots \\
X_{i}(q+1,K) & X_{i}(q+1,K) & \cdots & X_{i}(q+1,K) \\
X_{i}(i,k) & X_{i}(i,k) & \cdots & X_{i}(i,k) \\
\vdots & \vdots & \ddots & \vdots \\
X_{i}(I,K) & X_{i}(I,K) & \cdots & X_{i}(I,K)
\end{bmatrix}$$

(1)

where $X_{i}(i,k), X_{i}(i,k)$, and $X_{i}(i,k)$ represent data information in the time direction, batch direction, and the cross direction, which are defined as follows

$$X_{i}(i,k) = [x(i,k), x(i,k-1), \cdots x(i,k-p)]$$

$$X_{i}(i,k) = [x(i-1,k), x(i-2,k), \cdots x(i-q,k)]$$

$$X_{i}(i,k) = [x(i-1,k-1), \cdots x(i-q,k-p)]$$

(2)

As a result, the dimension of the augmented data matrix $X_{\text{aug}}$ is $(I-q+1)(K-p+1) \times pqJ$, where the column of $X_{\text{aug}}$ represents the measurement and the row of $X_{\text{aug}}$ contains the current process variables and the lagged ones through the time, batch and their cross directions.

2.2. Two-dimensional dynamic monitoring with SVDD

Suppose the original batch process dataset is given as $X(I \times J \times K)$, which can be unfolded into a two-dimensional dataset $X(I \times JK)$. To remove the mean trajectory of different batch process data, an auto-scaling step is carried out on the dataset $X(I \times JK)$, thus

$$\bar{X} = \frac{[X - \text{mean}(X)]}{\sigma(X)}$$

(3)

where $\text{mean}(\cdot)$ represents the mean value of the data matrix, and $\sigma(\cdot)$ is a calculator for the standard variance value of the data matrix. By introducing the dynamic steps in both of the time and batch directions, the augmented data matrix can be obtained through eqs. (1) and (2). Based on the augmented dataset $X_{\text{aug}}[(I-q+1)(K-p+1) \times pqJ]$, an SVDD model can be developed for process monitoring.

Since the nonlinear behavior has been assumed in the process, each data variable is firstly transformed from the original space to the feature space through a nonlinear function. Then, a hypersphere can be found in the feature space. By introducing a kernel function, the inner product of each two transformed data samples in the feature space can be represented as $K(x_{i}, x_{j}) = \langle \Phi(x_{i}), \Phi(x_{j}) \rangle$, where $i, j = 1, 2, \cdots (I-q+1)(K-p+1)$, $x_{i} = [X_{i}, X_{i}, X_{i}]$, $X_{i}, X_{i}, X_{i}$ are defined in eq.(2). In the present paper, the widely used Gaussian kernel function is employed for nonlinear SVDD modeling. To construct the minimum volume of the hypersphere, SVDD intends to solve the following optimization problem [Tax, and Duin, 1999]

$$\min_{\rho, \xi} R^{2} + C \sum_{i=1}^{n} \xi_{i}$$

s.t. $|\Phi(x_{i}) - a|^{2} \leq R^{2} + \xi_{i}, \xi_{i} \geq 0$ $i = 1, 2, \cdots, n$

(4)

where $a$ is the center of the hypersphere, $C$ gives the trade-off between the volume of the hypersphere and the number of errors. $\xi_{i}$ represents the slack variable which allows a probability that some of the training samples can be wrongly classified. Based on the quadratic optimization results of the SVDD model given in eq. (4), the center and the radius of the hypersphere can be calculated as follows [Tax, and Duin, 2004]
where $\mathbf{x}_i^{\text{neg}}$ is a support vector of the SVDD model, which lies in the surface of the hypersphere, $\alpha_i$ is the Lagrange multiplier of each data sample. The distance between the support vector and the center of the hypersphere is the radius of the hypersphere, which is given in eq. (6). In fact, only the support vectors have non-zero $\alpha$ values, the $\alpha$ value of any other data sample is zero. Therefore, the center of the hypersphere is actually a combination of support vectors of the SVDD model.

After the hypersphere has been found in the feature space, the normal region of the process can be enveloped by this hypersphere. As a result, a data sample should be considered as a normal one if its distance to the center of the hypersphere does not exceed the radius. Otherwise, the data sample will violate the modeling region of the SVDD method. Therefore, for batch process monitoring, a monitoring statistic which is based on the distance between the data sample and the center of the SVDD hypersphere can be defined as follow

$$\text{Dist} = d(\Phi(\mathbf{x}_i^{\text{neg}})) = \left| \Phi(\mathbf{x}_i^{\text{neg}}) - \mathbf{a} \right|$$

$$= \sqrt{1 - 2 \sum_{i=1}^{(l-q+1)(K-p+1)} \alpha_i K(\mathbf{x}_i^{\text{neg}}, \mathbf{x}_i^{\text{neg}}) + \sum_{i=1}^{(l-q+1)(K-p+1)} \sum_{j=1}^{(l-q+1)(K-p+1)} \alpha_i \alpha_j K(\mathbf{x}_i^{\text{neg}}, \mathbf{x}_j^{\text{neg}})}$$

The confidence limit of this distance based monitoring statistic is the radius of the hypersphere, by tuning the parameter $C$ in the SVDD model which control the tradeoff between the volume of the hypersphere and the classification error of the model, an appropriate confidence level can be determined. In the present work, the confidence level is selected as 99%. Therefore, if the distance of the data sample to the center of the hypersphere is small than the radius, it should be judged to be normal with a 99% confidence. In contrast, when the value of the monitoring statistic exceeds the control limit $\text{Dist} > R$, the data sample is judged to be abnormal, which means a fault has been detected in the batch process.

### 3. SIMULATION RESULTS

In this section, a simulation example is given for performance evaluation of the SVDD based two-dimensional dynamic batch process monitoring method, which is revised from the example used in reference [Lu et. al., 2005]. The dynamic relationships of the process variables are given as follows

$$x_i(i,k) = 0.8 * x_i(i-1,k) + 0.5 * x_i(i,k-1) - 0.33 * x_i(i-1,k-1) + v_1$$

$$x_i(i,k) = 0.44 * x_i(i-1,k) + 0.67 * x_i(i,k-1) - 0.11 * x_i(i-1,k-1) + v_2$$

$$x_i(i,k) = 0.65 * x_i^2(i,k) + 0.35 * x_i^2(i,k) + v_3$$

$$x_i(i,k) = -1.26 * x_i^2(i,k) + 0.33 * x_i^2(i,k) + v_4$$

where $i$ is the batch index, $k$ is the time index, $x_1$ and $x_2$ are two independent signals, $x_3$ and $x_4$ are nonlinear correlated with $x_1$ and $x_2$, $v_1, v_2, v_3, v_4$ are four Gaussian random signals with variance 0.01. The trajectories of $x_1$ and $x_2$ in the first batch are initialized by the following two first-order dynamic models

$$G_1(s) = \frac{0.8}{1+0.7s}$$

$$G_2(s) = \frac{0.6}{1+0.6s}$$

where $G_1(s)$ and $G_2(s)$ are transfer functions of the two dynamic models. Then, the first data sample of $x_1$ and $x_2$ in each of the following batch are set as $x_1(i,1) = x_1(i-1,1) + w_1$ and $x_2(i,1) = x_2(i-1,1) + w_2$, where $w_1$ and $w_2$ are independent Gaussian signals with variance 0.01.

For model training and testing purposes, a total of 30 batches are generated through eq. (8), each batch has 100 data samples. Among these 30 batches, 25 batches are used for modeling training, 5 batches are for testing. Based on the two-dimensional AIC rule, the dynamic orders of both two directions are determined as 2. Therefore, the dimension of the training data matrix is $2376 \times 16$. To examine the normality of each process variable, their distributions are compared with the standard Gaussian distribution, which are shown in Figure 1, where the red line represents the standard Gaussian distribution for each process variable. It can be seen that all of the four variables have violated the Gaussian assumption. Furthermore, the relationships between different process variables are nonlinear, which can be seen from eq. (8). Figure 2 shows the relationship between the third and fourth variables, clearly, the relation between these two variables is not linear. Therefore, the batch process data samples are not only non-Gaussian, but also nonlinear related.

To simulate the abnormal behavior in the batch process, the following three different cases are considered

**Case 1:**

$$x_1(i,k) = 0.65 * x_1^2(i,k) + 0.05 * x_1(i,k) + v_3$$

**Case 2:**

$$x_1(i,k) = -3.26 * x_1^2(i,k) + 0.33 * x_1^2(i,k) + v_4$$

**Case 3:**

$$x_1(i,k) = 0.44 * x_1(i-1,k) + 0.67 * x_1(i,k-1) - 0.11 * x_1(i-1,k-1) + 0.02 + v_5$$
where in the first case the relation between the third variable and the first two variables has been changed, and in the second case the coefficient -1.26 has been changed to -3.26 in the relationship between the fourth variable and the first variable. In the third abnormal case, a slight change of value 0.02 has been introduced to the second variable of the process. A total of 6 batches are generated in each of the three abnormal cases.

Figure 1: Gaussian testing of different process variables, (a) First variable; (b) Second variable; (c) Third variable; (d) Fourth variable.

Figure 2: Relationship between the third variable and the variable of the process

For construction of the SVDD model, the parameter of the Gaussian kernel function is selected as 50, and the value of the parameter C is determined as 0.08. The radius of the hypersphere in the feature space represents the 99% confidence level for the SVDD monitoring model. For comparison, a traditional two-dimensional dynamic PCA model is also built for batch process monitoring. In the previous two-dimensional dynamic PCA work, only the SPE statistic is incorporated for process monitoring, this is because the T2 statistic has violated the statistic assumption for process monitoring. Therefore, we only used the SPE monitoring statistic for performance comparison with the distance based monitoring statistic used in the present paper. First, the monitoring results of the abnormal batches in the first case are given in Figure 3. Although both of the two methods can successfully detect the change of the process, the detection rates of the SVDD based method is much higher than that of the PCA based method. However, PCA can hardly detect the abnormal behavior in the second case, while the SVDD based method can successfully detect this relation.
change. Both of these two monitoring results are presented in Figure 4. In the last case, a step change has been introduced to the second variable in each batch, which will generate a ramp change in the following abnormal batches. The monitoring results of the six abnormal batches in the third case are shown in Figure 5. It can be seen from Figure 5 (b) that PCA can only detect the fault in the last two abnormal batches, in which the change of the process is significant. However, the SVDD based monitoring statistic can detect the fault in all of the six batches, which are shown in Figure 5 (a). Therefore, based on the results of these three different abnormal cases, it can be inferred that the monitoring statistic based on the SVDD method is more sensitive for fault detection than the traditional PCA based monitoring statistic.
4. CONCLUSIONS

In the present paper, the SVDD method has been incorporated into the two-dimensional modeling framework for dynamic batch process monitoring. Compared to the two-dimensional PCA method, the SVDD based method has no Gaussian limitation of the process data, and the linear assumption of different process variables has also been extended to the nonlinear case. Based on the hypersphere constructed by the SVDD method, a monitoring statistic has been defined as the distance between the data sample and the center of the hypersphere. A simulation case study was provided to evaluate the efficiency of the proposed method, which has shown that the monitoring performance has been improved by the incorporation of the SVDD method.

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